

# Semidefinite programming characterization and spectral adversary method for quantum complexity with noncommuting unitary queries

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## Abstract

Generalizing earlier work characterizing the quantum query complexity of computing a function of an unknown classical “black box” function drawn from some set of such black box functions, we investigate a more general quantum query model in which the goal is to compute functions of  $N \times N$  “black box” unitary matrices drawn from a set of such matrices, a problem with applications to determining properties of quantum physical systems. We characterize the existence of an algorithm for such a query problem, with given query and error, as equivalent to the feasibility of a certain set of semidefinite programming constraints, or equivalently the infeasibility of a dual of these constraints, which we construct. Relaxing the primal constraints to correspond to mere pairwise near-orthogonality of the final states of a quantum computer, conditional on the various black-box inputs, rather than bounded-error distinguishability, we obtain a relaxed primal program the feasibility of whose dual still implies the nonexistence of a quantum algorithm. We use this to obtain a generalization, to our not-necessarily-commutative setting, of the “spectral adversary method” for quantum query lower bounds.

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## I. INTRODUCTION

Quantum computers can solve certain problems faster than any known classical algorithm: the best-known examples are probably Shor’s algorithm [1, 2] for factoring integers in time polynomial in the number of digits needed to represent them, and Grover’s “search” algorithm [3], which, for example, allows quadratic speedup (from time of order  $N$  to time of order  $\sqrt{N}$ ) of “brute-force search” for solutions to certain problems. The structure of these algorithms may be understood as based on “black-box” or “query” algorithms, in which we have as input a function implemented as a “black-box” subroutine, and we would like to determine a property of the black-box function with few calls ( “*queries*”) to the subroutine. For factoring, the corresponding query algorithm is one in which, given a strictly periodic function as a black-box, we must find its period[17]; for Grover’s, given a 0/1 valued function taking, say,  $n$ -bit strings as inputs, we must determine if the function is identically zero or not. In abstract models of such black-box computation, called “query models” by computer scientists, an instance of a problem is specified by a set of possible black-box functions, and a property of those functions (whose value, in some finite set, may depend on the function), which we want to compute with bounded error (say, less than some constant  $\varepsilon$ ). The *query complexity* of an instance is the minimal number of queries needed to compute the property on that instance. The cost of computation done between queries is ignored in this abstract model. Typically we are concerned with a problem having arbitrarily large instances, and with how the query complexity of instances scales with their size—for instance, polynomially in the case of the “order-finding” query problem [4] on which Shor’s algorithm is based, exponentially (but with half the classical exponent) in some versions of Grover’s algorithm. In concrete algorithms such as Shor’s factoring algorithm, or applications of Grover’s algorithm to speeding up the search for solutions to instances of hard problems, the black box is replaced by an explicit program or circuit, usually a polynomial time program or polynomial size circuit, but the algorithm treats it as a black-box, i.e. does not look at details of the program or circuit, but only provides inputs to it and processes outputs from it. Also, in such concrete algorithms based on black-box ones explicit algorithms must be provided for the computation that takes place between the queries, and this, too, is typically polynomial-time in input size. If the abstract black-box complexity of a problem is polynomial, *and* concrete algorithms can be founded implementing each black box polynomially, and each inter-box

computation polynomially, then the abstract black box algorithm can be converted into a concrete polynomial-time algorithm, as in the case of factoring. Lower bounds on black-box algorithms can imply lower bounds on the performance of concrete algorithms having such a substituted-black-box structure, but for these to be interesting, the possibility of known, easy ways of exploiting the structure of circuits in a concrete algorithm must be built in, for example by applying a lower bound technique to a set of queries including the inverse of the basic black-box transformations, if the circuit model allows (as does the standard quantum one) the easy construction of a polynomial-size circuit for the inverse of a given polynomial-size circuit. Likewise, the ability to apply a black box or not conditional on the value of some qubit should also be included for similar reasons (given a quantum circuit, it is easy to concoct another circuit of essentially the same size that applies the first conditionally). (This, and the point about the inverse, was suggested to me by Daniel Gottesman [5] at a talk I gave on an earlier version of this paper.)

In Grover’s algorithm, and many other abstract query algorithms such as the “Abelian hidden subgroup” problem that can be abstracted from Shor’s algorithm and its predecessors such as Simon’s algorithm [6], the black-boxes can be viewed as a set of commuting unitaries implementing “black-box functions” quantum-coherently. For example, they may compute a Boolean function  $f : \{1, \dots, S\} \mapsto \{0, 1\}$  of an input in  $\{1, \dots, S\}$  supplied in an  $S$ -dimensional quantum register in its “standard” or “computational” orthonormal basis  $|i\rangle, i \in \{1, \dots, S\}$ , and then write the resulting value onto an output qubit by adding it modulo 2 to the value of the output qubit in its standard basis  $\{|0\rangle, |1\rangle\}$ ; thus  $O_f|i\rangle|b\rangle = |i\rangle|f(i) \oplus b\rangle$ , for standard orthonormal bases of the two registers. For all the various possible such  $f$ , these “black-box” unitaries  $O_f$  commute with each other, being diagonal in the basis that is the product of the standard bases. Obviously, one can do something similar for a larger finite set of outputs. Other models for quantum queries to classical functions, such as “phase queries,”  $O_f|i\rangle \mapsto (-1)^{f(i)}|i\rangle$ , equivalent up to a constant factor in the number of queries to the above straightforward quantum-coherent reversible computation of  $f$  when conditioning and the adjoint unitaries are included, are sometimes used, and there too all unitaries commute.

In this paper, however, we analyze the case where queries involve a not-necessarily commuting set of black-box unitaries. This latter setting is relevant, for example, to algorithms intended to extract information about quantum physical systems, an area of intensive research. Although not all unitaries (e.g. on  $n$  qubits, a  $2^n$ -dimensional quantum system) can

be represented with polynomially many (in e.g.  $n$ ) quantum gates, the ones that can are still of great interest. Many interesting questions about unitaries are still superpolynomially hard (relative to  $P \neq NP$ ) when confined to such polynomially representable unitaries. Thus, just as in the case of “quantum-coherent classical” queries, there is the possibility that abstract query algorithms for determining properties of noncommuting quantum black-boxes may lead to efficient and important concrete algorithms.

Note, for example, that unitary evolutions induced by “local” hamiltonians on a lattice can be well approximated by polynomially many gates [7]. To extract certain information (e.g. about the spectrum) directly from the unitaries themselves involves manipulating  $2^n \times 2^n$  matrices. One could imagine using the short classical description of the small quantum circuit directly (i.e. in some way other than running the circuit, thereby going beyond the black-box model) to do the computation more quickly, even classically, but it is not clear that this will be possible and for certain problems, it is not possible in polynomial time unless  $P = NP$ . However, there is the tantalizing possibility that least some information may be gotten more efficiently than classically by treating the unitary as a “black box” in a quantum computation (legitimate in terms of actual computation time when it has a poly-size quantum circuit). Important candidate examples where the quantum algorithm is better than known classical ones include [8], [9], [10], [11].

An important part of the study of quantum computation has been the investigation of lower bounds on the quantum query complexity of various problems. Although lower bounds in query settings do not logically imply lower bounds of the same functional form for concrete versions of corresponding problems, because of the possibility of “looking inside the black box” in a concrete situation, many computer scientists view them as a good guide in many situations: for example, the lower bounds on Grover’s problem [12] matching the  $\sqrt{N}$  performance of Grover’s algorithm are widely taken as fairly reasonable grounds to expect that quantum computers will not perform NP-hard computations in polynomial time, although they are only part of the story as a crucial part of the question is whether one believes quantum circuits encoding classical computations may have some structure that quantum algorithms can take advantage of better than it is generally thought classical computations can take advantage of classical circuit structure.

In this paper, we provide a new formulation of the quantum query computation model with unitary black-box queries. It closely parallels the formulation for quantum-coherent

classical queries in [13]; all of the results in this paper have counterparts there and many of the ideas used in their proofs are related (indeed some parts are essentially identical) as well. As for quantum-coherent classical queries, our formulation takes the form of a theorem showing that a query algorithm for a problem instance exists if, and only if, a feasible solution to a certain set of semidefinite programming (SDP) constraints exists. This formulation contains, we think, the mathematical “essence” of quantum query complexity: much information concerning details of the unitaries implementing the between-query evolution in the standard picture, but irrelevant to the algorithm’s query complexity, is not present in our picture. The formulation allows us to derive space bounds for unitary query computations. It allows us to exploit the “revolution” of the last 15 years or so in conic, especially semidefinite, programming, leading to polynomial-time methods for solving these optimization problems, to obtain a polynomial algorithm for estimating the quantum query complexity of a problem instance.

## II. MATHEMATICAL AND NOTATIONAL PRELIMINARIES

In this next section, we will formalize two equivalent notions of quantum query algorithm, and use them to formally define quantum query complexity. First, however, we record some mathematical conventions, terminology, and facts we will use. We often define a set  $S$  as the set of all things referred to by some expression  $Expr(X)$  containing a variable, as the variable ranges over another set, say  $T$ ; we write this as:  $S := \{Expr(x)\}_{x \in T}$ . The pure states of quantum systems, which are vectors in a complex inner product space of finite dimension  $d$  (we’ll sometimes refer to it as a Hilbert space), will often be identified, usually without comment, with the isomorphic linear space of  $d \times 1$  matrices (“column vectors”) over  $\mathbb{C}$ , where the matrix is identified with the matrix elements of the state in some special basis. This special basis will be the basis used to define operators on that space. Thus the space of operators on a quantum space will also usually be implicitly identified with a space of matrices, and states, both pure and mixed, on tensor products of quantum spaces will also be identified with spaces of matrices, whose entries are interpreted as the operators’ matrix elements in the product of the standard bases for the individual spaces. Dirac notation will sometimes, but not exclusively, be used for vectors, or for projection operators, when especially when these represent, or directly correspond to, quantum states

of a query computer. We write  $M(d)$  for the space of  $d \times d$  complex Hermitian matrices.

The notion of “purification” of a mixed state  $\rho^{H_1}$  (operator on a Hilbert space  $H_1$ ) will also be used. This is a “pure” state  $|\Psi^{H_1 H_2}\rangle \in H_1 \otimes H_2$  such that  $\text{tr}_{H_2} |\Psi^{H_1 H_2}\rangle \langle \Psi^{H_1 H_2}| = \rho^{H_1}$ . We write  $d_i$  for the dimension of  $H_i$ ,  $i \in \{1, 2\}$ . It is a well known fact that *any* finite-dimensional positive semidefinite matrix  $\rho$  on  $H_1$  has a “purification” in  $H_1 \otimes H_2$  as long as  $d_2$  is at least  $\text{rank}(\rho)$ . A sometimes useful way of thinking about states on tensor products of spaces, and the partial trace, is in a block matrix picture: identifying the space of operators on  $H_1 \otimes H_2$  with the space of  $d_1 \times d_1$  block matrices with blocks in  $M(d_2)$  (viewed as arrays of matrix elements of the operator in the tensor product of standard bases for  $H_1, H_2$ ). Then the partial trace over  $H_1$  of a matrix  $M$  is the sum of its diagonal blocks, whereas its partial trace over  $H_2$  is the matrix of traces of its blocks. Parenthetical superscripts, like  $G^{(X,Y)}$ , indicate blocks of a block matrix.

Superscripts are used (as we have just done) to denote which system an operator acts on, or a vector belongs to (in the latter case they occur within the ket or bra notation), subscripts to index vectors or matrices belonging to an indexed set of such objects. “Functional” notation like  $|\Psi(t)\rangle$ ,  $\rho(t)$  also indicates dependence on an index, but its use will be confined to quantum states and variables directly related to quantum states, such as the variables in the “primal” semidefinite programs we define below, that correspond closely to quantum algorithms. The reason for this is that occasionally we want a quantum state to depend on which black box has been supplied to a quantum algorithm as “input”, and we reserve subscripts, as in  $|\Psi_X\rangle$ , to indicate this dependence on an input  $X$ . We often write, for example, the  $X, Y$  matrix element of  $G$  as  $G[X, Y]$ ; when an object is a quantum state, Dirac notation such as  $\langle X|G|Y\rangle$  may be used as well. Because of the other uses to which we put subscripts, they are never used to indicate matrix elements.

We use the notation  $|S|$  to indicate the cardinality of a set  $S$ . When a Hilbert space is defined in terms of a distinguished orthonormal basis indexed by a set  $S$  (i.e., defined as the free complex inner product space over the set  $S$ ), we may also use  $S$  to refer to the Hilbert space itself. Quite generally, we also write  $|S|$  for the dimension of a Hilbert space  $S$ ; there it does *not*, of course, refer to its cardinality.

### III. FORMULATION OF QUANTUM QUERY ALGORITHMS AND COMPLEXITY

We will use both a “black-box” and an equivalent “explicit input” model of quantum query complexity. In the black box model, a problem is given by specifying a set  $S$  of “black-box” unitary operators, a finite set  $T$ , and a function  $g : S \rightarrow T$ . The problem is to design an algorithm that, for all  $X \in S$ , computes  $g(X)$ , exactly or with zero or bounded error. We will mostly be interested in the bounded error case. The computer state will be written as a superposition of basis vectors  $|w\rangle|i\rangle \in Q \otimes W$ , where the first,  $n$ -dimensional, register  $Q$  is the “query register”, on which the unitary  $U \in S$  acts, and the second register,  $W$ , is workspace.

For what follows, we will let  $S$  be a finite set of unitaries in order to avoid having “matrices” indexed by infinite sets, or operators on infinite-dimensional spaces, though we expect generalizations to infinite sets of unitaries to be straightforward.

**Definition 1** *A finitary query problem instance in the unitary-queries model (problem for short) is an integer  $n$ , a finite set  $S$  of  $n \times n$  unitaries, a finite set  $T$ , and a function  $g : S \rightarrow T$ .*

**Definition 2** *A  $q$ -query quantum algorithm (QQA) for a problem  $P = (n, S, T, g)$  is an integer  $|W|$  (the “workspace dimension”), a sequence  $U_0, U_1, \dots, U_q$  of  $n|W| \times n|W|$  unitary matrices (the “inter-query unitaries”), and an indexed set of  $|T|$  projectors  $\{P_z\}_{z \in T}$ , that are  $n|W| \times n|W|$  matrices.*

On a black-box unitary input  $X$ , such an algorithm runs as follows. We consider a computer whose Hilbert space is  $Q \otimes W$ , the tensor product of an  $n$ -dimensional “query register”  $Q$  which has a distinguished orthonormal basis indexed by  $0, \dots, n-1$ , and a  $|W|$ -dimensional “workspace”  $W$  with a distinguished basis  $0, \dots, |W|-1$ . We define an action of the unitary matrices  $U_i$  on this space by interpreting them as the matrices of unitary operators  $Q \otimes W$  in an ordered basis  $|i\rangle|j\rangle$  (with the fast running index corresponding to  $Q$ ). We start with the computer state  $|0\rangle|0\rangle$ , and alternate the unitaries  $U_i$  with the fixed query unitary  $X$  (which acts only on the register  $Q$ , i.e. we apply  $X \otimes I$  to the computer). Thus at time  $t$  (immediately after the  $t$ -th query) the state of the computer when  $X$  is input is:  $|\phi_X(q)\rangle = U_t(X \otimes I)U_{t-1}(X \otimes I) \cdots U_1(X \otimes I)U_0|0\rangle|0\rangle$ . After  $q$  queries, the projectors

$\{P_z\}_z$  are measured, obtaining an outcome  $z \in T$ , interpreted as the value of  $g(X)$ , with probability

$$p(z) = \langle \Phi_X(q) | P_z | \Phi_X(q) \rangle . \quad (1)$$

The special case of computing a Boolean function  $f : \{0, 1\}^m \mapsto \{0, 1\}$  using phase queries corresponds to the commuting set of unitaries  $S = \{U_x\}_{x \in \{0, 1\}^m}$ , defined by  $\langle i | U_x | j \rangle = \delta_{ij} (-1)^{x_i}$ .

**Definition 3** *We say an algorithm  $A = (|W|, \{U_0, \dots, U_{q-1}\}, \{P_z\}_{z \in T})$  solves the problem  $P := (n, S, T, g)$  with bounded error  $\varepsilon$  (or for short,  $\varepsilon$ -computes  $g$ ), iff with  $|\phi_X(q)\rangle$  defined as above, for all  $z \in T$  and  $X \in S$  such that  $g(X) = z$ ,*

$$\langle \Phi_X(q) | P_z | \Phi_X(q) \rangle \geq \varepsilon . \quad (2)$$

We sometimes call such a QQA a “ $(q, \varepsilon)$ -QQA for  $g$ ”.

**Definition 4** *The quantum query complexity  $QQC_\varepsilon(g)$  of a function  $g$  is the least integer  $q$  such that there exists a  $q, \varepsilon$ -QQA for  $g$ .*

At times it will be useful to consider an “extended computer” whose Hilbert space is  $I \otimes Q \otimes W$ , with  $Q, W$  as before and  $I$  an  $|S|$ -dimensional “input” register with a distinguished orthonormal basis  $\{|X\rangle\}_{X \in S}$ . With such a construction, we can give an extended “explicit input” version of quantum query algorithms. The matrices  $X$  acting on  $Q$  are replaced by a single unitary matrix  $\Omega$  acting on  $I \otimes Q$  by “reading the input out of  $I$  in the standard basis” and, conditional on reading input  $X$ , doing the unitary  $X$  on the register  $Q$ . That is, in the tensor product basis  $|X\rangle|i\rangle$ ,  $\Omega$  acts via:

$$\Omega|X\rangle|i\rangle = |X\rangle X|i\rangle . \quad (3)$$

Thus the matrix  $\Omega$  written in this basis, with  $Q$ ’s basis the fast-running index, is block-diagonal, with the unitaries  $X$  as the diagonal blocks.

We can view the first  $t$  steps of an algorithm as acting on such a computer (starting in an initial state  $|\Psi^{IQW}\rangle$ ) to produce a state  $|\Psi^{IQW}(t)\rangle$  defined as follows:

**Definition 5**

$$|\Psi^{IQW}(t)\rangle := (I^I \otimes U_t^{QW})(\Omega^{IQ} \otimes I^W)(I^I \otimes U_{t-1}^{QW})(\Omega^{IQ} \otimes I^W) \dots (I^I \otimes U_1^{QW})(\Omega^{IQ} \otimes I^W)(I^I \otimes U_0^{QW})|\Psi^{IQW}\rangle . \quad (4)$$



Here we have introduced superscripts on unitaries to indicate which systems they act on, and superscripts inside kets to indicate the systems they belong to. These are not always used, however; sometimes we let the context make it clear what an operator acts on. Notice that the queries  $\Omega$  do not touch the workspace (and only touch the input register to read it in the standard basis), while the inter-query unitaries may arbitrarily entangle  $Q$  and  $W$ , but do not touch the “notional” input register  $I$ .

As we will see in the proof of the main theorem, some of the variables in the semidefinite program we will now define, and which appears in our first main theorem characterizing query complexity, can be interpreted as the density matrices of the subsystems  $I \otimes Q$  or  $I$  of such an extended query computer whose query and work registers are started in  $|0\rangle|0\rangle$ , and whose input register is started in an unnormalized equal superposition of inputs (so that  $|\Psi^{IQW}\rangle = \sum_{X \in S} |X\rangle|0\rangle|0\rangle$ ).

#### IV. SDP CHARACTERIZATION OF QUANTUM QUERY COMPLEXITY: PRIMAL FORMULATION

**Definition 6 (Semidefinite program  $P(g, q, \varepsilon)$ )** By  $P(g, q, \varepsilon)$  we mean the following semidefinite program feasibility problem: Find  $|S|n \times |S|n$  positive semidefinite Hermitian matrices  $\rho^{IQ}(t)$ ,  $t \in \{0, \dots, q-1\}$ , an  $|S| \times |S|$  PSD Hermitian matrix  $\rho^I(q)$  and  $|S| \times |S|$  PSD matrices  $\Gamma_z$ , for all  $z \in T$ , satisfying the constraints:

$$\text{tr}_Q \rho^{IQ}(0) = E \tag{5}$$

$$\text{tr}_Q \rho^{IQ}(t) = \text{tr}_Q \Omega \rho^{IQ}(t-1) \Omega^\dagger \tag{6}$$

for  $t \in \{0, \dots, q-1\}$ , where  $E$  is the constant all-ones matrix),

$$\rho^I(q) = \text{tr}_Q \Omega \rho^{IQ}(q-1) \Omega^\dagger, \tag{7}$$

$$\sum_{z \in T} \Gamma_z = \rho^I(q) \tag{8}$$

$$\Delta_z * \Gamma_z \succeq (1 - \varepsilon) \Delta_z, \tag{9}$$

where the constant diagonal matrix  $\Delta_z$  is defined by  $\Delta_z(X, X) = 1$  if  $g(X) = z$ , else 0.  $*$  denotes the elementwise (aka Schur or Hadamard) product of matrices.

Using this, we state the following theorem, which is the first main result of the paper:

**Theorem 1** *A  $q$ -query,  $\varepsilon$ -error quantum algorithm to compute  $g : S \rightarrow T$  exists if and only if a feasible solution to  $P(g, q, \varepsilon)$  does. Furthermore, for each particular feasible solution  $\langle \{\rho^{IQ}(t)\}_t, \rho^I(q), \{\Gamma_z\}_{z \in T} \rangle$  there is a  $(q, \varepsilon)$ -QQA that computes  $g$ , for which the dimension  $r$  of the working memory is no larger than the greater of  $|S|N$  and  $\lceil \sum_{z \in T} \text{rank}(\Gamma_z)/N \rceil$ . Since the latter is no greater than  $\lceil |S||T|/N \rceil$ , it follows that any  $(q, \varepsilon)$ -QQA computing  $g$  may be implemented with workspace dimension no greater than  $\max |S|N, \lceil |S||T|/N \rceil$  in addition to the  $N$ -dimensional query register.*

In terms of qubits, then, the algorithm needs no more than  $\max \{ \lceil \log |S| \rceil + \lceil \log N \rceil, \lceil \log |S| \rceil + \lceil \log |T| \rceil \} - \lfloor \log N \rfloor$  qubits of workspace in addition to the  $\lceil \log N \rceil$ -qubit query register.

**Proof:** We prove first the implication from the existence of a  $(q, \varepsilon)$ -QQA solving the problem to the existence of a feasible solution to  $P(g, q, \varepsilon)$ , establishing it by constructing the latter from the former. We do this by defining matrices  $\rho^{IQ}(t)$ ,  $\Gamma_z$  in terms of the objects of the QQA, and showing that they satisfy the constraints (5–9) on the variables of the same names in the definition of  $P(g, q, \varepsilon)$ .

We begin by showing that in order to tell whether an algorithm will succeed in  $\varepsilon$ -computing the function  $g$  no matter what the input, *all* we need to know is whether the geometry (the inner products) of the final computer states  $|\Phi_X^{QW}(q)\rangle$  allows these states to, roughly (i.e. up to  $\varepsilon$ ), lie in a set of orthogonal subspaces such that the vectors  $|\Phi_X^{QW}\rangle$  in each subspace share the same value of  $g(X)$ . (They may have to be isometrically embedded in a larger space to do this.) Formally, this gives an SDP which we now construct. We array the inner products in a matrix  $G(q)$  defined

**Definition 7**  $\tilde{M}(q)[X, Y] := \langle \Phi_X^{QW}(q) | \Phi_Y^{QW}(q) \rangle$ .

For later use, similar matrices  $G(t)$  may be defined for all  $t$  between 0 and  $q$  inclusive, using the conditional computer states  $|\Psi^{IQW}(t)\rangle$  after the  $t$ -th query and post-query unitary. The  $t = 0$  case, before any query, is of course the all-ones matrix. Because these are matrices of inner products (sometimes called “Gram matrices”), they are necessarily positive semidefinite. The condition that the geometry of the final inner products is correct may be stated as a semidefinite programming feasibility problem with a constraint involving  $G(q)$ :

**Definition 8 (SDP  $O(g, \varepsilon, M)$ )** For a problem  $g$ , real number  $\varepsilon$  between zero and one, and  $|S| \times |S|$  positive semidefinite matrix  $M$ , the program  $O(g, \varepsilon, M)$  is the following: Find  $|S| \times |S|$  PSD matrices  $\{\Gamma_z\}_{z \in T}$  such that

$$\sum_{z \in T} \Gamma_z = G \quad (10)$$

$$\Delta_z * \Gamma_z \succeq (1 - \varepsilon) \Delta_z. \quad (11)$$

The proof of the following lemma essentially repeats part of the proof of the main theorem in [13].

**Lemma 1** The SDP  $O(g, \varepsilon, G(q))$ , where  $G(q)$  is defined as in Definition 7 above to be the final-state inner-products matrix of a QQA for  $g$ , is feasible if the QQA  $\varepsilon$ -computes  $g$ .

**Proof of lemma:** The feasible solution is obtained by defining  $\Gamma_z$  as the matrices with components:

$$\Gamma_z[X, Y] := \langle \Phi_X^{QW}(q) | P_z | \Phi_X^{QW}(q) \rangle. \quad (12)$$

Satisfaction of the constraint (10) follows because  $\sum_z P_z = I$ , while (11) is guaranteed by Eq. (2) in Definition 3. ■

The definition of  $\Gamma_z$  just given is also the one will use to show feasibility of  $P(q, \varepsilon)$ .

Lemma 1 has a suitable converse (see below). Thus to decide, from the final inner-products matrix  $G(q)$ , whether the value of  $g$  has been  $\varepsilon$ -computed or not, is a question of semidefinite program feasibility. However, essentially because the action of the queries is not linear on the matrices  $G(t)$  that we defined based on the QQA (the inner-product matrices of the input-conditioned states after query  $t$ ), we cannot formulate linear constraints on variables corresponding to  $G(t)$  that enforce the condition that the final inner-products matrix must arise from the initial one via queries and pre- and post-query unitaries. We need different, though related, quantities to formulate that condition as a linear constraint.

These quantities are most easily and intuitively described by going to the “explicit inputs” formulation described above, with overall state space  $IQW$  including the “virtual input register”  $I$  started in an unnormalized uniform superposition of inputs. It is easily seen, using the definitions of  $\Omega$ ,  $|\Psi_X^{QW}(t)\rangle$ , and  $|\Psi^{IQW}(t)\rangle$ , that

$$|\Psi^{IQW}(t)\rangle = \sum_{X \in S} |X^I\rangle |\Phi_X^{QW}(t)\rangle. \quad (13)$$

We define  $\rho^{IQW}(t) := |\Psi^{IQW}(t)\rangle\langle\Psi^{IQW}(t)|$ , and density matrices such as  $\rho^{IQ}(t) := \text{tr}_W \rho^{IQW}(t)$ , etc.... It is then easily seen by direct calculation that

$$\langle X|\rho^I(t)|Y\rangle = \langle\Phi_X(t)|\Phi_Y(t)\rangle, \quad (14)$$

and consequently that the matrix of  $\rho^I(t)$  in the standard basis that labels inputs, is just the Gram matrix  $G(t)$  of Definition 7. We will generally identify operators with their matrices in the standard tensor product basis for  $IQW$ , and hence if the QQA  $\varepsilon$ -computes  $g$ , the program  $O(g, \varepsilon, \rho^I(q))$  with  $\rho^I(q) := \text{tr}_Q[\rho^{IQ}(q)]$  in place of  $M$ , is feasible. Moreover, the quantities  $\rho^{IQ}(t)$  are exactly those necessary to formulate the computational constraints linearly, as we now show.

Since in our analysis we will at times consider separately the effects of the query and of the post-query unitary, we also define  $|\Phi_X^{QW}(t+)\rangle := (X^Q \otimes I^W)|\Phi_X^{QW}(t)\rangle$ ,  $|\Phi^{IQW}(t+)\rangle := (\Omega^{IQ} \otimes I^W)|\Phi^{IQW}(t)\rangle$ , and  $\rho^{IQ}(t+)$  as the “density” matrix  $\text{tr}_W[|\Psi^{IQW}(t+)\rangle\langle\Psi^{IQW}(t+)\rangle]$ ; these are the vectors and density matrix after the  $t$ -th query but before the  $t$ -th post-query unitary. Since the post-query unitary  $U^{QW}(t)$  does not touch  $I$ ,  $\rho^I(t) = \rho^I((t-1)+)$ , or in other words:

$$\text{tr}_Q \rho^{IQ}(t) = \text{tr}_Q \rho^{IQ}((t-1)+). \quad (15)$$

Since the query is just the implementation of the unitary  $\Omega$  on  $IQ$ , we have:

$$\rho^{IQ}((t-1)+) = \Omega \rho^{IQ}(t-1) \Omega^\dagger. \quad (16)$$

Eliminating the unnecessary quantities  $\rho^{IQ}((t-1)+)$ , we can combine the two preceding sets of equations into a single set (indexed by  $t$ ) of linear equations:

$$\text{tr}_Q \rho^{IQ}(t) = \text{tr}_Q \Omega \rho^{IQ}(t-1) \Omega^\dagger. \quad (17)$$

In other words, the quantities  $\rho^{IQ}(t)$  satisfy the constraints (6). It is also clear that  $\rho^{IQ}(0)$  as defined from the algorithm satisfies (5), because  $U^{QW}(0)$  does not touch  $I$ , and  $|\Psi^{IQW}\rangle$  has the all-ones matrix as its reduced density matrix. Furthermore, since as stated in Eq. (14),  $G(t) \equiv \rho^I(t)$  and the latter is just  $\text{tr}_Q \rho^{IQ}(t)$ , we have from Lemma 1 and its proof that  $\Gamma_z$  as defined in that proof satisfy the constraints (8) and (9). Thus we have shown the first direction of the theorem (existence of a QQA implies feasible solution to the SDP).

It remains to show the other direction, that the existence of a feasible solution for  $P(g, q, \varepsilon)$  implies that of an  $\varepsilon$ -QQA solving the problem with the stated amount of workspace. Again

it is a straightforward construction, though we must keep track of the amount of workspace used in the algorithm we construct. In this part of the proof  $\rho^{IQ}(t)$ ,  $\Gamma_z$  will be taken to be the feasible values of the variables of the same names in Definition 6; it will turn out, of course, that when we have constructed the desired QQA, they will coincide with the quantities of the same names,  $\rho^{IQ}(t)$ ,  $\Gamma_z$ , obtainable from that QQA via the definitions in the first part of our proof.

The construction begins with a converse of Lemma 1.

**Lemma 2** *If the SDP  $O(g, \varepsilon, M)$ , has feasible solution  $\{\Gamma_z\}_{z \in T}$  there exists a set of vectors  $\{|\Psi_X\rangle\}_{X \in T}$  in a Hilbert space of dimension no greater than  $\sum_{z \in T} \text{rank}(\Gamma_z) \leq |S||T|$  and projectors  $P_z$  acting on that space such that  $M$  is the Gram matrix of  $\{|\Psi_X\rangle\}_{X \in T}$  and  $P_z$  satisfy Eqs. (12) and (2).*

**Sketch of proof of Lemma 2:** The proof (with notational differences) may be found in [13]; it proceeds by constructing vectors  $|\Theta_X\rangle$  of length  $|S|$  and a “POVM” consisting of  $|S| \times |S|$  PSD matrices  $\{R_z\}_{z \in T}$  such that  $\sum_{z \in T} R_z = I$  and  $\langle \Theta_X | R_z | \Theta_X \rangle \geq \varepsilon$ , and then Naimark-extending the POVM to a set of projectors  $P_z$  in a larger space and identifying  $|\Psi_X\rangle$  as the corresponding embeddings of the vectors  $|\Theta_X\rangle$  in the larger space. This ensures that  $|\Psi_X\rangle$  satisfy (2). The minimal dimension required for the Naimark extension is  $\sum_{z \in T} \text{rank}(\Gamma_z)$ . ■

Since Eqs. (8) and (9) just state that  $O(q, \varepsilon, M)$  with  $\text{tr}_Q \rho^{IQ}(q)$  substituted for  $M$  is satisfied, Lemma 2 gives us vectors  $\{|\Psi_X(q)\rangle\}_{X \in T}$  in a Hilbert space  $H$  of dimension  $|H| := \sum_{z \in T} \text{rank}(\Gamma_z)$  whose Gram matrix is  $\text{tr}_Q(\rho^{IQ}(q))$  and projectors  $P_z$  on that space, which together satisfy Eqs. (12) and (2). We may give  $H$  the structure  $Q \otimes W$  with  $Q$   $|S|$ -dimensional and the dimension of  $W$  large enough to guarantee that  $\dim(Q \otimes W) \geq \sum_{z \in T} \text{rank}(\Gamma_z)$ ;  $|W| = \lceil |H|/|N| \rceil \leq \lceil |S||T|/|N| \rceil$  suffices. Given the vectors  $|\Psi_X(q)\rangle \in Q \otimes W$ , we can construct the state  $|\Psi^{IQW}\rangle := \sum_X |X^I\rangle |\Psi_X^{QW}(q)\rangle$ . By construction, this state’s reduced density matrix for system  $I$  will equal the feasible  $\rho^I(q)$ .

Now suppose we have  $|\Psi^{IQW}(t)\rangle$  such that its reduced density matrix coincides with the feasible value  $\rho^{IQ}(t)$  (or, for the case  $t = q$ , some arbitrary  $\rho^{IQ}(t)$  whose  $I$  density matrix coincides with the feasible  $\rho^I(q)$ ). We construct  $U^{QW}$  such that  $|\Psi^{IQW}(t-1)\rangle := (\Omega^{IQ\dagger} \otimes I^W)(I^I \otimes U^{QW\dagger})|\Psi^{IQW}(t)\rangle$ , has  $IQ$  reduced density matrix equal to  $\rho^{IQ}(t-1)$  (or, for the case  $t = 1$ , to the all-ones matrix). To do this, first note that any purification of  $\Omega \rho^{IQ}(t-1) \Omega^\dagger$  into

$W$  (and there exist many so long as  $|W| \geq |I||Q|$ ) is also a purification of  $\rho^I(t) := \text{tr}_Q \rho^{IQ}(t)$  into  $QW$ , by the constraint (6). Moreover, by acting via a unitary  $U^{QW\dagger}$  on  $|\Psi^{IQW}(t)\rangle$ , we can reach such a purification of  $\rho^I(t)$  that is also a purification of  $\Omega \rho^{IQ}(t-1) \Omega^\dagger$ , as long as  $W$  has dimension at least  $|S|N$ . We let a  $U^{QW}$  that achieves this be the  $t$ -th unitary,  $U^{QW}(t)$  of our algorithm, and define  $|\Psi^{IQW}(t-1)\rangle := (\Omega^{IQ\dagger} \otimes I^W)(I^I \otimes U^{QW\dagger})|\Psi^{IQW}(t)\rangle$ . Thus,  $\text{tr}_Q |\Psi^{IQW}(t-1)\rangle \langle \Psi^{IQW}(t-1)| = \rho^{IQ}(t-1)$ , as claimed.

We apply this step beginning with the states  $|\Psi^{IQW}(q)\rangle$  already constructed, until we get state  $|\Psi^{IQW}(0)\rangle$  which by construction will have the all-ones matrix as its reduced density matrix, and thus  $|\Psi^{IQW}(0)\rangle = \sum_X |X\rangle |\chi^{QW}\rangle$ , where WLOG we can choose  $U^{QW}(0)$  so that  $U^{QW\dagger}(0) |\chi^{QW}\rangle = |0\rangle$ . Thus the sequence  $U^{QW}(0), \dots, U^{QW}(q)$ , and the indexed set  $\{P_z\}_{z \in T}$  we have constructed are a quantum algorithm that  $\varepsilon$ -computes  $g$ , and the dimension of  $W$  satisfies the claimed bound, which derives from the bounds on  $|Q \otimes W|$  of  $\sum_z \text{rank}(\Gamma_z)$  (from the Naimark extension at the output) and  $|S|N$  (from the workspace needed to reach an arbitrary purification of a fixed  $\rho^{IQ}$  in the post-query unitary step).  $\blacksquare$

**Remark:** For those who like the matrix picture, thinking of the matrix  $G(t)$  of  $\rho^{IQ}(t)$  in the standard basis blocked according to  $X$  and  $Y$ , we see that during the query each block is updated according to a fixed block-dependent linear map:

$$G^{(X,Y)} \mapsto YGX^\dagger. \quad (18)$$

This is just conjugation by the block-diagonal unitary matrix whose  $(X, X)$  block is  $X$  (i.e., the matrix of  $\Omega$ ).

Using this we can express the constraints (6) in terms of the matrix  $M$  viewed as blocked according to  $X, Y$ . Each of the  $q$  constraints on the matrices  $\rho^{IQ}(t)$  (which states that an  $|S| \times |S|$  matrix calculated from  $\rho^{IQ}$ , namely its partial trace  $\rho^I$ , is equal to another such matrix), becomes  $\frac{|S|(|S|+1)}{2}$  constraints each stating that the trace of an  $(X, Y)$  block of some matrix is equal to that of another:

$$\text{tr} [G^{(X,Y)}(t)] = \text{tr} [YG^{(X,Y)}(t-1+)X^\dagger], \quad (19)$$

or, in the case  $t = q$ , a similar set of constraints with no trace on the LHS. This is because the matrix of the partial trace in question is the matrix of traces of the blocks; since the block matrix is Hermitian, only  $|S|(|S|+1)/2$  blocks, say those on and above the main diagonal of blocks, are independent. Equivalently,

$$\text{tr} [G^{(X,Y)}(t)] = \text{tr} [X^\dagger Y G^{(X,Y)}(t-1+)]. \quad (20)$$

■

## V. THE DUAL SDP

In order to find the SDP feasibility problem dual to the one just given, we begin by stating a very general theorem concerning feasibility of conic program constraint sets.

**Theorem 2** *Let  $K$  be a closed, pointed, generating convex cone in an  $m$ -dimensional real vector space  $V$ , with a distinguished inner product  $(\cdot, \cdot)$ . Let  $W$  be a  $p$ -dimensional real vector space, also equipped with a distinguished inner product (written similarly). Let  $K^* \subset V$  be the cone dual to  $K$  according  $V$ 's inner product. Let  $A$  be a fixed linear transformation from  $V$  to  $W$  whose kernel is  $\{0\}$ , and let  $b \in W$  be a constant nonzero vector. Let  $A^* : W \rightarrow V$  be the linear map “dual” or “adjoint” to  $A$ , defined by  $(w, Av) = (A^*w, v)$ . (For example, if  $V$  and  $W$  are viewed as spaces of column vectors of lengths  $m$  and  $p$  respectively equipped with the inner products  $(u, v) = u^t v$ , and  $A$  is represented by its  $p \times m$  matrix  $\hat{A}$ , then  $A^*$ 's matrix is  $\hat{A}^t$ .)*

*Consider the conic programming feasible set defined by:*

$$P := \{x \in V : Ax = b, x \geq_K 0\}, \quad (21)$$

*This set is empty (the constraints are “infeasible”) if and only if the dual feasible set*

$$D := \{y \in W : A^*y \geq_{K^*} 0, (b, y) < 0\} \quad (22)$$

*is nonempty (the dual constraints are “feasible”).*

**Proof:** First let  $x$  belong to  $P$ . Suppose that  $A^*y \in K^*$ , so  $y$  satisfies the first condition defining  $D$ . We show that  $(b, y) \geq 0$ , so that  $y \notin D$ .  $A^*y \in K^*$  implies (since  $x \in K$ ) that  $(x, A^*y) \geq 0$ . Thus  $(Ax, y) \geq 0$ ; since  $x \in P$ ,  $Ax = b$ , so  $(b, y) \geq 0$ .

Next, supposing  $P$  infeasible we construct a point in  $D$ . Consider the  $A$ -image of  $K$ , denoted  $AK$ . By the assumption that  $A$ 's kernel is  $\{0\}$ , and for example Theorem 9.1 of [14],  $AK$  is a closed convex cone. Now,  $b \notin AK$ , for if it were, its preimage would belong to  $P$ , contradicting the supposition. Therefore, by (for example) Theorems 11.1, 11.3, and 11.7 of [14], there exists a hyperplane through the origin properly separating  $b$  and  $AK$ ; this hyperplane is the zero-set of a linear functional  $L(x) := (y, x)$  determined by a vector

$y \in W$ . Thus (cf. the proof of Thm. 11.1 in [14])  $(b, y) < 0$ , and for all  $z \in AK$ ,  $(z, y) \geq 0$ . The latter is equivalent to: for all  $x \in K$ ,  $(Ax, y) \equiv (x, A^*y) \geq 0$ . Thus  $y \in D$ .  $\blacksquare$

Lemma 2 of [13] was a special case of this, for a particular cone  $K$  and a particular form of the linear map  $A$ . In [13] we then further specialized the Lemma to the case in which the primal feasible set  $P$  was the SDP characterizing the existence of a quantum query algorithm for classical Boolean queries. We now proceed by giving a generalization of Lemma 2 of [13] which is still a special case of the above theorem, but which is sufficiently general to encompass the SDP characterizing quantum query complexity with arbitrary queries.

**Lemma 3** *Let  $K \subset W$  be the product of  $k$  cones of PSD Hermitian matrices (with the  $r$ -th cone a cone of  $d_r \times d_r$  matrices), in the obvious  $W$  (direct sum of the spaces of  $d_r \times d_r$  Hermitian matrices). Let  $V$  be the direct sum of  $k$  copies of  $H(s)$  for some fixed  $s$ . Let  $\mathbf{A}$  be a fixed  $k \times k$  matrix whose entries are linear maps  $\mathcal{A}_{\alpha,\beta} : H(d_\beta) \mapsto H(s)$ . Let  $\mathbf{B}$  be a nonzero element of  $V$ , i.e. a  $k$ -tuple of matrices  $B_\beta$ , with  $B_\beta \in H(s)$ . Equip  $V$  and  $W$  with the trace inner products,  $(A, B) := \text{tr } AB$ . (Matrices in  $V$  and  $W$  are block-diagonal,  $k$  blocks by  $k$  blocks.) Consider the “primal” feasible set:*

$$P := \{X \in W : \sum_{\beta} \mathcal{A}_{\alpha\beta}(X_\beta) = B_\alpha, X \in K\} , \quad (23)$$

and the “dual” feasible set

$$D := \{Y \in V : \sum_{\beta} \mathcal{A}_{\beta\alpha}^*(Y_\beta) \geq_K 0, \sum_{\beta} \text{tr } Y_\beta B_\beta < 0\} . \quad (24)$$

Suppose further that the only feasible solution to  $P_0$  (the primal problem with  $B_\alpha$  set equal to zero) is  $0 \in W$ . Then if  $D$  is feasible,  $P$  is infeasible, and vice versa.

We caution the reader not to confuse the variable matrices  $X_\alpha, Y_\beta$  appearing in the SDP above with the variables  $X$  and  $Y$  that we commonly let range over input unitaries in  $S$ . We will rarely use these notations together, and only when it is clear from the context what is meant, and in any case we never use subscripts on the input unitaries, nor do we ever omit subscripts from the primal and dual variables of the above type of program.

**Remark:** Note that  $\mathcal{A}^*$  is the linear map often called by quantum information theorists  $\mathcal{A}^\dagger$ , defined by  $\text{tr } F\mathcal{A}^\dagger(G) = \text{tr } \mathcal{A}(F)G$  (for all  $F$  in the input space and  $G$  in the output space,



though it suffices to require it for bases of these spaces given linearity). In the case where  $\mathcal{A}$  is completely positive, i.e.  $\mathcal{A} : G \mapsto \sum_i A_i G A_i^\dagger$ ,  $\mathcal{A}^\dagger$  may be defined via  $\mathcal{A}^\dagger : G \mapsto \sum_i A_i^\dagger G A_i$ . ■

The program  $P(g, \varepsilon, q)$  is a case of  $P$ , for which  $W$  is the direct sum of  $q$  copies of  $H(|S|n)$  and  $2|T| + 1$  copies of  $H(|S|)$ , and  $V$  is the direct sum of  $q + 2 + |T|$  copies of  $H(|S|)$ . In terms of the associated query algorithm, the  $q$  copies of  $H(|S|n)$  in  $W$  are where the density matrices  $\rho^{IQ}(t)$  will live, one of the copies of  $H(|S|)$  is for  $\rho^I(q)$  and the other  $2|T|$  copies of  $H(|S|)$  are for the the output conditions:  $|T|$  of them, indexed by  $z \in T$ , for an additive decomposition of the final  $\rho^I$  into positive matrices  $\Gamma_z$  representing the portion of the output matrix for which the final measurement has result  $z$ , and  $|T|$  more for slack variable matrices  $\Pi_z$ , used to transform the inequality conditions on the  $\Gamma_z$ , for succesful computation, into equality conditions. These inequality conditions are  $\Delta_z * \Gamma_z \succeq (1 - \varepsilon) \Gamma_z$ ; requiring the slack variables  $\Pi_z$  to be positive while enforcing the equality constraint  $\Delta_z * \Gamma_z - \Pi_z = (1 - \varepsilon) \Delta_z$  is equivalent to imposing the inequality constraint on the  $\Gamma_z$ . Thus the vector of primal variables  $X_\beta$  is indexed as follows: for  $0 \leq \beta \leq q - 1$ ,  $X_\beta = \rho^{IQ}(\beta)$ ; for  $\beta = q$ ,  $X_\beta = \rho^I(q)$ ; for  $\beta = q + z (z \in T \equiv \{1, \dots, |T|\})$ ,  $X_\beta = \Gamma_z$ ; for  $\beta = q + 1 + |T| + z (z \in T \equiv \{1, \dots, |T|\})$ ,  $X_\beta = \Pi_z$ .

We now specify the maps  $\mathcal{A}_{\alpha, \beta}$  and constant vector  $\mathbf{B} = [B_\alpha]$ . We will give rows of the matrix  $\mathcal{A}_{\alpha, \beta}$ , followed by the corresponding RHS constant  $B_\alpha$ , since each row and  $B_\alpha$  corresponds to a constraint; the constraints will be naturally grouped by type.

For  $0 \leq \alpha \leq q - 1$ ,  $\mathcal{A}_{\alpha, \alpha}$  is the partial trace map  $G^{IQ} \mapsto \text{tr}_Q(G^{IQ})$ , and (for  $1 \leq \alpha \leq q$ )  $\mathcal{A}_{\alpha-1, \alpha} : G^{IQ} \mapsto -\text{tr}_Q(G^{IQ})$ , with the rest of the maps zero for  $\alpha, \beta$  in this range. The corresponding RHS constants are  $B_0 = E$  (where  $E$  is the all-ones matrix in  $H(|S|)$ ), and  $B_\alpha = 0$  ( $1 \leq \alpha \leq q$ ); thus far we have imposed all the trace constraints on query-updating (constraints  $0, \dots, q - 1$  give the effect of the pre-query unitary and query, while constraint  $q$  gives the effect of the unitary following the last query).  $\mathcal{A}_{q+1, q}$  is minus the identity map, while  $\mathcal{A}_{q+1, q+z}$ , for  $z \in |T|$ , is the identity map  $\text{id} : X \mapsto X$  (and the other maps  $\mathcal{A}_{q+1, x}$  are zero). The corresponding RHS constants are zero: this imposes the constraint that the  $\Gamma_z$  are an additive decomposition of  $\rho^I(q)$  into positive matrices. Finally, for  $\alpha = q + 1 + z, z \in |T|$ ,  $\mathcal{A}_{\alpha, q+z} : X \mapsto \Delta_z * X$ ,  $\mathcal{A}_{\alpha, q+1+z+|T|} = -\text{id}$ , and the rest of them are zero. And the corresponding RHS constants,  $B_\alpha : \alpha = q + 1 + z, z \in T$ , are zero matrices. These just impose the output conditions, in the equality-constraint form with slack variables

given above.

To make this clearer, we display in Appendix B the constraints in the form  $Ax = b$ , where  $A$  is the matrix of maps  $A_{\alpha\beta}$ ,  $x$  and  $b$  are column vectors of matrices  $X_\alpha$ ,  $B_\beta$ ; we also display there the dual matrix-multiplication part of the dual constraints. Appendix B serves as a useful aid to verifying that the procedure about to be described for deriving the dual of  $P(g, \varepsilon, q)$  is carried out correctly, and that problem  $D(g, \varepsilon, q)$  below is the result.

The dual feasible set is obtained, using Theorem 2, by transposing the matrix of maps, and replacing each map with its dual. When  $\mathcal{A} : I \otimes Q \rightarrow I$  is the partial trace map, its dual  $\mathcal{A}^* : I \rightarrow I \otimes Q$  is given by  $\mathcal{A}^* : L \mapsto L \otimes I$  (where, to clear up ambiguous notation,  $I$  in this last specification refers to the identity matrix on the system  $Q$ , not to the system  $I$  itself as it does in the preceding two). For  $\mathcal{A} : G \mapsto \text{tr}_Q(\Omega G \Omega^\dagger)$ , we have  $\mathcal{A}^* : L \mapsto \Omega^\dagger(L \otimes I)\Omega$ .

**Remark:** We can give more explicit forms of these maps (and incorporate the special form of  $\Omega$ , in the second case). Viewing elements of  $I \otimes Q$  as block matrices blocked according to  $X, Y \in S$ , and elements of  $I$  as matrices with elements indexed by pairs  $X, Y \in S$ , we have, when  $\mathcal{A}$  is the partial trace map, that  $\mathcal{A}^*$  takes  $M$  to the matrix whose blocks are  $M_{XY}I$ . For  $\mathcal{A}^* : G \mapsto \Omega^\dagger(M \otimes I)\Omega$ , the output matrix is the one whose blocks are  $M_{XY}Y^\dagger X$ . It is of course dual to itself, and so, as is easily verified, are the maps  $M \mapsto \Delta_z * M$ . ■

We thus obtain a version of the dual program  $D(g, \varepsilon, q)$ . The dual variables are  $q+1+|T|$   $|S| \times |S|$  Hermitian matrices  $Y_\beta$  whose matrix elements are indexed by input-pairs  $(X, Y) \in S \times S$ . The first  $q$ , corresponding to the primal query updating constraints, we call  $L_t$ , ( $t \in \{0, \dots, q-1\}$ ); the next, corresponding to the primal constraint that the  $\Gamma_z$  add up to  $\rho^I(q)$ , we call  $L_q$ ; and the last  $|T|$ , each corresponding to the output constraint on a primal variable  $\Gamma_z$ , we call  $\Lambda_z (z \in T)$ . We must find such matrices satisfying the constraints:

$$L_{(t-1)} \otimes I - \Omega^\dagger(L_t \otimes I)\Omega \succeq 0 \quad (1 \leq t \leq q) \quad (25)$$

$$L_q = L_{q+1} \quad (26)$$

$$L_{q+1} \succeq -\Delta_z * \Lambda_{z+1}, \quad (1 \leq z \leq |T|) \quad (27)$$

$$-\Lambda_z \preceq 0 \quad (1 \leq z \leq |T|) \quad (28)$$

$$\sum_{X,Y \in S} (L_0)_{X,Y} + (1 - \varepsilon) \text{tr} \sum_{z \in T} \Delta_z * \Lambda_z < 0. \quad (29)$$

Redefining the  $\Lambda_z$  to be the negatives of the  $\Lambda_z$  above, so as to have them be PSD, changing some signs, and dropping the redundant variable  $L_{q+1}$ , we formally define the dual

program:

**Definition 9** *The semidefinite program (feasibility problem)  $D(g, \varepsilon, q)$  is defined as the problem of finding  $q+1$   $|S| \times |S|$  Hermitian matrices  $L_q, q \in \{0, \dots, q\}$  and  $|T|$   $|S| \times |S|$  Hermitian matrices  $\Lambda_z$  for  $z \in T$ , with matrix elements indexed by  $S \times S$ , such that:*

$$L_{(t-1)} \otimes I \succeq \Omega^\dagger(L_t \otimes I)\Omega^\dagger \quad (1 \leq t \leq q) \quad (30)$$

$$L_q \succeq \Delta_z * \Lambda_z, \quad (1 \leq z \leq |T|) \quad (31)$$

$$\Lambda_z \succeq 0 \quad (1 \leq z \leq |T|) \quad (32)$$

$$\sum_{X,Y \in S} (L_0)_{X,Y} < (1 - \varepsilon) \sum_{z \in T} \sum_{X:g(X)=z} (\Lambda_z)_{X,X} . \quad (33)$$

Comparison to the program  $\hat{P}(f, t, \varepsilon)$  of Theorem 2 in [13] shows that they are identical except for the first constraint (the query-updating one), and that when  $\Omega$  has the special form corresponding to classical phase queries to input strings  $x$  (when  $x$  is in the input register), then  $D$  above specializes to  $\hat{P}$  of [13].

Note that the constraint (30) says that the block matrix whose  $X, Y$  block is the  $N \times N$  matrix  $L_t[X, Y]X^\dagger Y - L^{t-1}[X, Y]I$  is positive semidefinite.

An immediate consequence of Theorem 1 and 3, is the following Theorem.

**Theorem 3** *With  $S, T$  as above, a  $q$ -query,  $\varepsilon$ -error quantum algorithm to compute  $g : S \rightarrow T$  exists if and only if a feasible solution to  $D(g, q, \varepsilon)$  does not.*

## VI. RELAXATION, DUALITY, AND A GENERALIZED SPECTRAL ADVERSARY METHOD

### A. Relaxation to the pairwise output condition: primal and dual programs

We now consider relaxing the primal program by substituting the weaker output condition of “pairwise near-orthogonality,” also known as the “Ambainis condition” [15]:

$$|\rho^I(q)[X, Y]| \leq 2\sqrt{\varepsilon(1 - \varepsilon)} \text{ when } g(X) \neq g(Y) . \quad (34)$$

We call it “pairwise near-orthogonality” because, by (14), when  $\rho^{IQ}(q)$  is viewed as the unnormalized density matrix of the input register in the explicit-inputs model,  $|\rho^{IQ}(q)[X, Y]|$

is the modulus of the inner product of the  $QW$  computer states conditional on inputs  $X$  and  $Y$  in the “black-box” model, so it states that these conditional states are nearly (for small  $\varepsilon$ ) orthogonal if  $X$  and  $Y$  have different values of  $g$ ; a necessary, but not sufficient, condition for them to be the final states in a successful computation of  $g$ .

In order to formulate this as a semidefinite constraint, we need constant matrices  $V^{XY} \in M(|S|)$ , for all *unordered* pairs  $(X, Y)$  of  $X, Y \in S$  such that  $g(X) \neq g(Y)$  (we call this set  $\tilde{R}$  for future reference). For each such pair we define  $V^{XY}$  to be the matrix whose  $X, Y$  and  $Y, X$  matrix elements are 1, and whose other matrix elements are all zero. We also need the constant matrices  $W^{XY}$  for the same unordered input-pairs, but whose  $X, X$  and  $Y, Y$  matrix elements are 1 (and whose others are zero). Then the Ambainis output condition is equivalent to the conditions:

$$V^{XY} * \rho^I(q) + 2\sqrt{\varepsilon(1-\varepsilon)}W^{XY} \succeq 0 \quad (35)$$

where  $(X, Y) \in R$ . We won't need the output variables  $\Gamma_z$  in this case, but we will need a slack variable  $\Pi^{XY} \succeq 0$  for each of the  $|R|$  unordered pairs, to get equality constraints

$$V^{XY} * \rho^I(q) + 2\sqrt{\varepsilon(1-\varepsilon)}W^{XY} = \Pi^{XY}. \quad (36)$$

Thus the dual program is to find  $|S| \times |S|$  Hermitian matrices  $L^t$ ,  $0 \leq t \leq q$  and  $\Upsilon_{XY}$ ,  $X, Y \in S$ , such that:

$$L_{t-1} \otimes I \succeq \Omega(L_t \otimes I)\Omega^\dagger \quad (1 \leq t \leq q) \quad (37)$$

$$L_q \succeq \sum_{(X,Y) \in R} (V^{XY} * \Upsilon_{XY}) \quad (38)$$

$$\Upsilon_{X,Y} \succeq \mathbf{0} \quad (X, Y) \in R \quad (39)$$

$$\sum_{X,Y \in S} L_0[X, Y] < -2\sqrt{\varepsilon(1-\varepsilon)} \sum_{(X,Y) \in R} \text{tr}(\Upsilon^{XY} W^{XY}), \quad (40)$$

and  $(\Upsilon_{XY})_{MN} = 0$  unless  $MN \in \{XX, XY, YX, YY\}$ .

Rewriting this in terms of the variables  $K_t := -L_{q-t}$  we formally define the dual program  $D_A$ .

**Definition 10**

$$K_0 \preceq - \sum_{(X,Y) \in R} (V^{XY} * \Upsilon_{XY}) \quad (41)$$

$$K_{t-1} \otimes I \preceq \Omega(K_t \otimes I) \Omega^\dagger \quad (1 \leq t \leq q) \quad (42)$$

$$\Upsilon_{X,Y} \succeq \mathbf{0} \quad ((X,Y) \in R) \quad (43)$$

$$\sum_{X,Y \in S} K_q[X,Y] > 2\sqrt{\varepsilon(1-\varepsilon)} \sum_{(X,Y) \in R} \text{tr } \Upsilon^{XY}, \quad (44)$$

and  $(\Upsilon_{XY})_{MN} = 0$  unless  $MN \in \{XX, XY, YX, YY\}$ .

## B. A generalized spectral adversary method

We next obtain, from this dual program, a generalization of Theorem 4 of [13], giving a lower bound directly on the number of queries in an algorithm  $\varepsilon$ -computing a function, in terms of relatively easily computed properties of the function and a “weight matrix”  $\Gamma$  that we are free to choose. This gives a generalization of the so-called “spectral adversary method” for quantum query complexity lower bounds. We use the notation  $\lambda(M)$  for the largest eigenvalue of a matrix  $M$ .

**Theorem 4** *Let  $S$  be a finite set of unitary  $|S| \times |S|$  matrices, and let  $g : S \mapsto T$ ,  $T$  a finite set. Let  $\Gamma$  be a nonnegative real symmetric  $|S| \times |S|$  matrix indexed by  $S$ , such that  $\Gamma_{X,Y} = 0$  whenever  $g(X) \neq g(Y)$ . Then*

$$QQC_\varepsilon(g) \geq \frac{(1 - 2\sqrt{\varepsilon(1-\varepsilon)})\lambda(\Gamma)}{2\lambda(\Gamma \otimes I - \Omega(\Gamma \otimes I)\Omega^\dagger)}. \quad (45)$$

**Proof:** To prove this, we construct, for any  $\Gamma$  as above and  $q$  below the bound given in the theorem, a sequence  $K_t : 0 \leq t \leq q$ ,  $\Upsilon_{XY}, \{X,Y\} \in R$  that is a feasible solution to  $D_A(g, q, \varepsilon)$ .

Note that by the standard Perron-Frobenius theory of nonnegative matrices [16],  $\Gamma$  has a normalized eigenvector  $v$  with nonnegative entries, whose eigenvalue is  $\Gamma$ ’s largest, i.e.  $\lambda(\Gamma)$ . We define  $K_t := (\Gamma - t\alpha I) * vv^t$ , where  $\alpha := 2\lambda(\Gamma \otimes I - \Omega(\Gamma \otimes I)\Omega^\dagger)$ . We also define  $\Upsilon_{XY}$  via

$$\begin{aligned} \Upsilon_{XY}[X,X] &= \Upsilon_{XY}[Y,Y] = -\Upsilon_{XY}[X,Y] = -\Upsilon_{XY}[Y,X] := \\ &K_0[X,Y] \equiv \Gamma[X,Y]v[X]v[Y], \end{aligned} \quad (46)$$

with its other matrix elements zero. These are manifestly positive semidefinite, satisfying (43). That (41) is satisfied with equality is also immediate from the definitions.

To verify that (42) is satisfied, we have a look at

$$\Omega(K_t \otimes I)\Omega^\dagger - K_{t-1} \otimes I = \Omega((\Gamma - t\alpha I) * vv^t) \otimes I \Omega^\dagger - ((\Gamma - (t-1)\alpha I) * vv^t) \otimes I \quad (47)$$

$$= (vv^t \otimes E) * \Omega(\Gamma - t\alpha I) \otimes I \Omega^\dagger - (vv^t \otimes E) * ((\Gamma - (t-1)\alpha I) \otimes I) \quad (48)$$

$$= (vv^t \otimes E) * [\Omega(\Gamma \otimes I)\Omega^\dagger - t\alpha(I \otimes I) - \Gamma \otimes I + (t-1)\alpha(I \otimes I)] \quad (49)$$

$$= (vv^t \otimes E) * [\Omega(\Gamma \otimes I)\Omega^\dagger - \Gamma \otimes I - \alpha(I \otimes I)] . \quad (50)$$

Note that in the second equality we used the identity

$$Z^\dagger(X * M \otimes I)Z \equiv (M \otimes E) * Z^\dagger(X \otimes I)Z , \quad (51)$$

which does not hold for general  $Z$ , but does hold when (as in the cases  $Z = \Omega, Z = I$  that we use)  $Z$  is block-diagonal when the blocks are indexed by a basis for the input register (the register that we write on the left in tensor products). The matrix in (50) is positive semidefinite by the definition of  $\alpha$ , so the constraint (42) is indeed satisfied. Finally, the constraint (44) is satisfied because

$$\sum_{(X,Y) \in R} \text{tr } \Upsilon_{XY} = \sum_{(X,Y) \in R} 2\Gamma[X,Y]v[X]v[Y] = v^t \Gamma v = \lambda(\Gamma) , \quad (52)$$

while  $\sum_{XY} K_q[X,Y] = \lambda(\Gamma) - q\alpha$ , which by our assumption on  $q$  is greater than or equal to  $2\sqrt{\varepsilon(1-\varepsilon)}\lambda(\Gamma)$ . ■

It is easily seen that this Theorem specializes to Theorem 4 of [13].

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## APPENDIX A: THE MATRIX MULTIPLICATIONS APPEARING IN THE PRIMAL AND DUAL CONSTRAINTS

In this section we use the notation  $\text{tr}_Q$  to denote the partial trace map from  $I \otimes Q$  to  $I$ ,  $\Omega$  to denote the map  $G \mapsto \Omega G \Omega^\dagger$ ,  $\Delta_k^*$  to denote the map  $G \mapsto \Delta_k * G$  (where  $*$  is the elementwise matrix product); juxtaposition of maps to indicate composition (thus  $\text{tr}_Q \Omega : G \mapsto \text{tr}_Q(\Omega G \Omega^\dagger)$ ), and the superscript  $*$  to indicate the dual map. We also use the facts that the maps  $\Delta_k^*$  are self-dual and that the dual  $\Omega^*$  of the map  $\Omega$  is the map  $\Omega^\dagger : M \mapsto \Omega^\dagger M \Omega$ .

## 1. Unrelaxed constraints

With this notation, the matrix multiplication portion of the primal constraints is:

$$\left( \begin{array}{c|c|c} \begin{array}{ccc} \text{tr}_Q & & \\ -\text{tr}_Q \Omega & \text{tr}_Q & \\ & \ddots & \ddots \\ & & -\text{tr}_Q \Omega & \text{id} \end{array} & & \\ \hline & -\text{id} & \begin{array}{cccc} \text{id} & \text{id} & \cdots & \text{id} \end{array} \\ \hline & & \begin{array}{cccc} \Delta_1^* & & & \\ & \Delta_2^* & & \\ & & \ddots & \\ & & & \Delta_{|T|}^* \end{array} \end{array} \right) \begin{bmatrix} \rho^{IQ}(0) \\ \rho^{IQ}(1) \\ \vdots \\ \rho^{IQ}(q-1) \\ \hline \rho^I(q) \\ \hline \Gamma_1 \\ \Gamma_2 \\ \vdots \\ \Gamma_{|T|} \\ \hline \Pi_1 \\ \vdots \\ \Pi_{|T|} \end{bmatrix} = \begin{bmatrix} E \\ \mathbf{0} \\ \vdots \\ \mathbf{0} \\ \hline \mathbf{0} \\ (1-\varepsilon)\Delta_1 \\ (1-\varepsilon)\Delta_2 \\ \vdots \\ (1-\varepsilon)\Delta_{|T|} \end{bmatrix} \quad (\text{A1})$$

The matrix multiplication part of the dual constraints is:

$$\left( \begin{array}{c|c|c} \begin{array}{ccc} \text{tr}_Q^* & -\Omega^\dagger \text{tr}_Q^* & \\ & \text{tr}_Q^* & -\Omega^\dagger \text{tr}_Q^* \\ & & \ddots & \ddots \\ & & & \text{tr}_Q^* & -\Omega^\dagger \text{tr}_Q^* \\ & & & & \text{id} \end{array} & & \\ \hline & -\text{id} & \begin{array}{c} \text{id} \\ \vdots \\ \text{id} \end{array} \\ \hline & & \begin{array}{ccc} \Delta_1^* & & \\ & \ddots & \\ & & \Delta_{|T|}^* \end{array} \end{array} \right) \begin{bmatrix} L_0 \\ L(1) \\ \vdots \\ L_q \\ \hline L(q+1) \\ \hline \Lambda_1 \\ \Lambda_2 \\ \vdots \\ \Lambda_{|T|} \end{bmatrix} \succeq \begin{bmatrix} \mathbf{0} \\ \vdots \\ \mathbf{0} \\ \hline \mathbf{0} \\ \vdots \\ \mathbf{0} \\ \hline \mathbf{0} \\ \vdots \\ \mathbf{0} \end{bmatrix} \quad (\text{A2})$$

## 2. Relaxed constraints (pairwise output condition)

Primal matrix multiplication constraints:

$$\left( \begin{array}{ccc|cc} \text{tr}_Q & & & & \\ -\text{tr}_Q \Omega & \text{tr}_Q & & & \\ & \ddots & \ddots & & \\ & & -\text{tr}_Q \Omega & \text{tr}_Q & \\ & & -\text{tr}_Q \Omega & & \\ \hline & & & \text{id} & \\ \hline & & -V_{X_1, Y_1}^* & \text{id} & \\ & & -V_{X_2, Y_2}^* & & \text{id} \\ & & \vdots & & \ddots \\ & & & & \text{id} \end{array} \right) \begin{bmatrix} \rho^{IQ}(0) \\ \rho^{IQ}(1) \\ \vdots \\ \rho^{IQ}(q) \\ \hline \rho^I(q) \\ \Pi_{X_1, Y_1} \\ \Pi_{X_2, Y_2} \\ \vdots \\ \Pi_{X_{|R|}, Y_{|R|}} \end{bmatrix} = \begin{bmatrix} E \\ \mathbf{0} \\ \vdots \\ \mathbf{0} \\ \mathbf{0} \\ \hline 2\sqrt{\varepsilon(1-\varepsilon)}W_{X_1, Y_1} \\ 2\sqrt{\varepsilon(1-\varepsilon)}W_{X_2, Y_2} \\ \vdots \\ 2\sqrt{\varepsilon(1-\varepsilon)}W_{X_{|R|}, Y_{|R|}} \end{bmatrix} \quad (\text{A3})$$

From the above we get the dual matrix multiplication constraints:

$$\left( \begin{array}{ccc|cccc} \text{tr}_Q^* & -\Omega^\dagger \text{tr}_Q^* & & & & \\ & \text{tr}_Q^* & -\Omega^\dagger \text{tr}_Q^* & & & \\ & & \ddots & \ddots & & \\ & & & \text{tr}_Q^* & -\Omega^\dagger \text{tr}_Q^* & \\ \hline & & & \text{id} & -V_{X_1, Y_1}^* & \cdots & -V_{X_{|R|}, Y_{|R|}}^* \\ \hline & & & & \text{id} & & \\ & & & & & \ddots & \\ & & & & & & \text{id} \end{array} \right) \begin{bmatrix} L_0 \\ L(1) \\ \vdots \\ L_q \\ \hline \Upsilon_1 \\ \Upsilon_2 \\ \vdots \\ \Upsilon_{X_{|R|}, Y_{|R|}} \end{bmatrix} \preceq \begin{bmatrix} \mathbf{0} \\ \vdots \\ \mathbf{0} \\ \hline \mathbf{0} \\ \mathbf{0} \\ \vdots \\ \mathbf{0} \end{bmatrix} \quad (\text{A4})$$

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